

Temperature optimization problems governed by semi-discrete phase-field models of grain boundary motions

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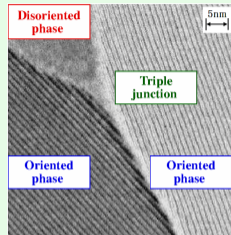
0. Kobayashi–Warren–Carter type system of grain boundary motion

$0 < T < \infty$, $\Omega \subset \mathbb{R}^N$: b.d.d. domain ($N \in \{1, 2, 3, 4\}$), $\Gamma = \partial\Omega$: smooth, n_Γ : unit outer normal, $Q := (0, T) \times \Omega$

KWC system: cf. [Kobayashi–Warren–Carter](2000)

$$\begin{cases} \partial_t \eta - \Delta \eta + g(\eta) + \alpha'(\eta) |\nabla \theta| = u(t, x), & (t, x) \in Q, \\ \alpha_0(\eta) \partial_t \theta - \operatorname{div} \left(\alpha(\eta) \frac{D\theta}{|D\theta|} + \nu^2 \nabla \theta \right) = v(t, x), & (t, x) \in Q, \\ \nabla \eta \cdot n_\Gamma = 0, \quad \theta = 0 \text{ on } \Sigma := (0, T) \times \Gamma, \\ \eta(0, x) = \eta_0(x), \quad \theta(0, x) = \theta_0(x), \quad x \in \Omega. \end{cases}$$

- $\eta = \eta(t, x)$: orientation order ($\eta \geq 1$: oriented, $\eta \leq 0$: disoriented),
- $\theta = \theta(t, x)$: orientation angle of grain
- $u = u(t, x)$: temperature, $v = v(t, x)$: forcing for θ
- $g \in C^2(\mathbb{R})$: Lipschitz, $\exists G \in C^3(\mathbb{R})$ s.t. $G' = g$ on \mathbb{R}
- $0 < \alpha \in C^2(\mathbb{R})$: convex • $\alpha_0 \in W_{\text{loc}}^{1, \infty}(\mathbb{R})$: fixed function
- $[\eta_0, \theta_0] = [\eta_0(x), \theta_0(x)]$: fixed initial data of $[\eta, \theta]$ • $\nu > 0$: fixed constant



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The Gradient system of free-energy:

$$[\eta, \theta] \mapsto \mathcal{F}(\eta, \theta) := \frac{1}{2} \int_{\Omega} |\nabla \eta|^2 dx + \int_{\Omega} G(\eta) dx + \int_{\Omega} \left(\alpha(\eta) |\nabla \theta| + \frac{\nu^2}{2} |\nabla \theta|^2 \right) dx.$$

◇ Sketch of history

[1] Existence and large-time behavior

- (*) the case of $\nu > 0$: [Ito–Kenmochi–Yamazaki](2008–2011)
the results in active case of $\nu \Delta \theta$
- (**) the case of $\nu = 0$: [Moll–S.–Watanabe](2011–)
the results in very singular case of $-\operatorname{div}\left(\alpha(\eta) \frac{D\theta}{|D\theta|}\right)$

[2] Uniqueness (a few, and only in the case of $\nu > 0$)

- (i) 1D-case of Ω : [Ito–Kenmochi–Yamazaki](2008)
- (ii) η -independent case of $\alpha_0 \partial_t \theta = \alpha_0(t, x) \partial_t \theta$: [Antil–Kubota–S.–Yamazaki](2020–)
 Ω is higher dimensional, but $0 < \alpha_0 \in W^{1,\infty}(Q)$ (positive, b.d.d., Lipschitz)

[3] Optimal control problem ($\nu > 0$)

- (iii) continuation work of (ii): [Antil–Kubota–S.–Yamazaki](2020–)
Existence, parameter dependence of optimal controls, **necessary condition of optimality**

This talk: Optimal control problem under η -dependent case of $\alpha_0 \implies$ time-discrete setting

1. Time-discrete Kobayashi–Warren–Carter type system of grain boundary motion

$\Omega \subset \mathbb{R}^N$: b.d.d. domain ($N \in \{1, 2, 3, 4\}$), $\Gamma = \partial\Omega$: smooth, n_Γ : unit outer normal

$$n \in \mathbb{N}, \tau = T/n \text{ (time-step-size)} \quad X := L^2(\Omega), \quad \mathbb{X} := [X]^n$$

State-system (S)₀: cf. [Moll–S.–Watanabe](2014–)

$$\begin{cases} \frac{1}{\tau}(\eta_i - \eta_{i-1}) - \Delta\eta_i + g(\eta_i) + \alpha'(\eta_i)|\nabla\theta_{i-1}| = u_i \text{ in } \Omega, & \text{(1st.eq)} \end{cases}$$

$$\begin{cases} \frac{1}{\tau}\alpha_0(\eta_{i-1})(\theta_i - \theta_{i-1}) - \operatorname{div}\left(\alpha(\eta_i)\frac{D\theta_i}{|D\theta_i|} + \nu^2\nabla\theta_i\right) = v_i \text{ in } \Omega, & \text{(2nd.eq)} \end{cases}$$

$$\begin{cases} \nabla\eta_i \cdot n_\Gamma = 0, \quad \theta_i = 0 \text{ on } \Gamma, i = 1, 2, 3, \dots, n, \\ \eta_0 \in H^1(\Omega), \quad \theta_0 \in H_0^1(\Omega). \end{cases}$$

- $\eta = \{\eta_i\}_{i=1}^n \in \mathbb{X}$: orientation order
- $\theta = \{\theta_i\}_{i=1}^n \in \mathbb{X}$: orientation angle of grain
- $u = \{u_i\}_{i=1}^n \in \mathbb{X}$: temperature, $v = \{v_i\}_{i=1}^n \in \mathbb{X}$: forcing for θ

†₁. The state system (S)₀ is a coupled system of **two schemes of minimizing movements**: (1st.eq) and (2nd.eq)

†₂. The coupled minimizing movements can be solved **separately**, in the order of (1st.eq) → (2nd.eq)

2. Temperature constrained optimal control problem

$\Omega \subset \mathbb{R}^N$, $\Gamma := \partial\Omega$: (smooth), $X := L^2(\Omega)$, $\mathbb{X} := [X]^n$

Problem (OP)₀: find $[u^*, v^*] = [\{u_i^*\}_{i=1}^n, \{v_i^*\}_{i=1}^n] \in [\mathbb{X}]^2$, called **optimal control**, s.t.

$$[u^*, v^*] = \arg\text{-min} \mathcal{J} = \mathcal{J}(u, v) \text{ on a constrained class } \mathcal{U}_{\text{ad}},$$

with a cost functional $\mathcal{J} : [u, v] \in [\mathbb{X}]^2 \mapsto \mathcal{J}(u, v) \in [0, \infty)$, defined as

$$\mathcal{J}(u, v) := \frac{1}{2} |[\eta, \theta] - [\eta_{\text{ad}}, \theta_{\text{ad}}]|_{[\mathbb{X}]^2}^2 + \frac{1}{2} |[u, v]|_{[\mathbb{X}]^2}^2.$$

In the context,

- $u = \{u_i\}_{i=1}^n$: the control for $\eta = \{\eta_i\}_{i=1}^n$ (temperature), $v = \{v_i\}_{i=1}^n$: the control for $\theta = \{\theta_i\}_{i=1}^n$
- $[\eta, \theta] = [\{\eta_i\}_{i=1}^n, \{\theta_i\}_{i=1}^n] \in [\mathbb{X}]^2$: the solution to the state-system (S)₀, for any $[u, v] \in [\mathbb{X}]^2$.
- $[\eta_{\text{ad}}, \theta_{\text{ad}}] = [\{\eta_{\text{ad},i}\}_{i=1}^n, \{\theta_{\text{ad},i}\}_{i=1}^n] \in [\mathbb{X}]^2$: the admissible target profile for $[\eta, \theta]$
- \mathcal{U}_{ad} : a class of **admissible controls** $[u, v] \in [\mathbb{X}]^2$, which fulfill:
 - **box-constraint**: $\sigma_{*,i} \leq u_i \leq \sigma_i^*$ a.e. in Ω , $i = 1, 2, 3, \dots, n$, with fixed obstacle sequences $\sigma_* := \{\sigma_{*,i}\}_{i=1}^n, \sigma^* = \{\sigma_i^*\}_{i=1}^n \in [L^\infty(\Omega)]^n$

†₁. The time-discrete setting can be applied to the **numerical scheme**, directly

3. Approximating problems

Problem (OP) $_{\varepsilon}$ with $\varepsilon \geq 0$: find $[u^*, v^*] = [\{u_i^*\}_{i=1}^n, \{v_i^*\}_{i=1}^n] \in [\mathbb{X}]^2$, called **optimal control**, s.t.

$$[u_{\varepsilon}^*, v_{\varepsilon}^*] = \arg\text{-min} \mathcal{J}_{\varepsilon} = \mathcal{J}_{\varepsilon}(u, v) \text{ on a constrained class } \mathcal{U}_{\text{ad}},$$

with a **regularized cost functional** $\mathcal{J}_{\varepsilon} : [u, v] \in [\mathbb{X}]^2 \mapsto \mathcal{J}_{\varepsilon}(u, v) \in [0, \infty)$, defined as

$$\mathcal{J}_{\varepsilon}(u, v) := \frac{1}{2} |[\eta_{\varepsilon}, \theta_{\varepsilon}] - [\eta_{\text{ad}}, \theta_{\text{ad}}]|_{[\mathbb{X}]^2}^2 + \frac{1}{2} |[u, v]|_{[\mathbb{X}]^2}^2.$$

State-system (S) $_{\varepsilon}$:

$$\begin{cases} \frac{1}{\tau}(\eta_{\varepsilon, i} - \eta_{\varepsilon, i-1}) - \Delta \eta_{\varepsilon, i} + g(\eta_{\varepsilon, i}) + \alpha'(\eta_{\varepsilon, i}) f_{\varepsilon}(\nabla \theta_{\varepsilon, i-1}) = u \text{ in } \Omega, \\ \frac{1}{\tau} \alpha_0(\eta_{\varepsilon, i-1})(\theta_{\varepsilon, i} - \theta_{\varepsilon, i-1}) - \text{div}(\alpha(\eta_{\varepsilon, i}) \partial f_{\varepsilon}(\nabla \theta_{\varepsilon, i}) + \nu^2 \nabla \theta_{\varepsilon, i}) \ni v \text{ in } \Omega, \\ \nabla \eta_{\varepsilon, i} \cdot n_{\Gamma} = 0, \quad \theta_{\varepsilon, i} = 0 \text{ on } \Gamma, \\ \eta_{\varepsilon, 0}(x) = \eta_0(x), \quad \theta_{\varepsilon, 0}(x) = \theta_0(x), \quad x \in \Omega. \end{cases}$$

• $f_{\varepsilon}(\omega) := \sqrt{\varepsilon^2 + |\omega|^2}$, $\forall \omega \in \mathbb{R}^N$, $\varepsilon > 0$ ($f_{\varepsilon} \rightarrow f_0 := |\cdot|$ in $L^{\infty}(\mathbb{R}^N)$ as $\varepsilon \downarrow 0$)

$\partial f_{\varepsilon} \subset \mathbb{R} \times \mathbb{R}$: **subdifferential of f_{ε}** ($\partial f_0(\nabla \theta) \sim$ “set-valued sign function” $\sim \frac{\nabla \theta}{|\nabla \theta|}$)

4. Main Theorems

Former part: mathematical analysis by means of calculus of variation

Theorem A. Existence and parameter-dependence of optimal controls for $\varepsilon \geq 0$

Theorem B. The first order necessary condition in the case of $\varepsilon > 0$ (regular case of the problem $(OP)_\varepsilon$)

Keypoint: linearization method for the state-system \iff Gâteaux differential of the cost

$$\begin{array}{l} \text{quasilinear diffusion in } (S)_\varepsilon \\ -\operatorname{div}\left(\alpha(\eta) \frac{\nabla\theta}{\sqrt{\varepsilon^2 + |\nabla\theta|^2}}\right) \end{array} \longrightarrow \begin{array}{l} \text{diffusion in the necessary condition} \\ -\operatorname{div}\left(\alpha(\eta) \frac{(\varepsilon^2 + |\nabla\theta|^2)I - \nabla\theta \otimes \nabla\theta}{\sqrt{\varepsilon^2 + |\nabla\theta|^2}^3} \nabla v\right) \\ (v \in \mathbb{X}: \text{component of optimal control}) \end{array}$$

Theorem C. The limiting observation of the necessary condition as $\varepsilon \downarrow 0$

Keypoint: limiting approach to the singular case of the problem $(OP)_0$

$$\begin{array}{l} \text{singular diffusion in } (S)_0 \\ -\operatorname{div}\left(\alpha(\eta) \frac{D\theta}{|D\theta|}\right) \end{array} \longrightarrow \boxed{\zeta^\circ \in [\mathcal{D}'(\Omega)]^n (?)}$$

Latter part: precise observation under 1D-setting of $\Omega = (0, 1)$

Theorem D. Limiting necessary condition, on some neighborhood of the grain boundary

Keypoint: H^2 -regularity of solutions to $(S)_0$

Decomposition property of quasilinear diffusion: $-\partial_x\left(\alpha(\eta) \frac{D\theta}{|D\theta|}\right) + \nu^2 \partial_x \theta = -\partial_x\left(\alpha(\eta) \frac{D\theta}{|D\theta|}\right) - \nu^2 \partial_x^2 \theta$ in \mathbb{X}

Assumptions and notations.

(A0) $N \in \{1, 2, 3, 4\}$, $\nu > 0$, $\sigma_* = \{\sigma_{*,i}\}_{i=1}^n$, $\sigma^* = \{\sigma_i^*\}_{i=1}^n \in [L^\infty(\Omega)]^n$; $\sigma_{*,i} \leq \sigma_i^*$ a.e. in Ω , $i = 1, \dots, n$,

$$X := L^2(\Omega), \mathbb{X} := [X]^n, Y := H^1(\Omega), \mathbb{Y} := [Y]^n, Y_0 := H_0^1(\Omega), \mathbb{Y}_0 := [Y_0]^n$$

(A1) $\alpha_0 \in W_{\text{loc}}^{1,\infty}(\mathbb{R})$ and $\alpha_0 > 0$ on $\bar{\Omega}$.

(A2) $\alpha \in C^2(\mathbb{R})$, s.t. $\alpha'(0) = 0$, $\alpha'' \geq 0$, and $\delta_\alpha := \inf \alpha(\mathbb{R}) \cup \alpha_0(\mathbb{R}) > 0$

(A3) $g \in C^2(\mathbb{R})$: **Lipschitz**, having a non-negative potential $0 \leq G \in C^3(\mathbb{R})$, and there exist constants $-\infty < r_* \leq 0 < r^* < \infty$, which satisfy:

$$\begin{cases} g(\eta_i) \leq -|\sigma_{*,i}|_{L^\infty(\Omega)}, \text{ for } \eta_i \leq r_*, \text{ for any } i = 1, 2, 3, \dots, n, \\ g(\eta_i) \geq |\sigma_i^*|_{L^\infty(\Omega)}, \text{ for } \eta_i \geq r^*, \text{ for any } i = 1, 2, 3, \dots, n. \end{cases}$$

(A4) $[\eta_0, \theta_0] \in [Y \cap L^\infty(\Omega)] \times Y_0$, and $r_* \leq \eta_0 \leq r^*$ a.e. in Ω

(A5) Let $n \in \mathbb{N}$ be a large number, s.t.:

$$0 < \tau = \frac{T}{n} < \frac{\nu^2}{4(\nu^2(1 + |g'|_{L^\infty(\mathbb{R})}) + |\alpha'|_{L^\infty(\mathbb{R})})}$$

- †₁• The conditions colored blue are for the L^∞ -boundedness of the orientation order $\eta = \{\eta_i\}_{i=1}^n \in \mathbb{X}$
- †₂• The assumption (A5) is for the **strict coercivity** (existence and uniqueness) of $(S)_\varepsilon$

Proposition 1 (Solvability of the state-system $(S)_\varepsilon$) cf. [Moll–S.–Watanabe](2013–)

Let us assume (A0)–(A5). Then, for $\varepsilon \geq 0$, and $[u, v] \in \mathcal{U}_{\text{ad}}$, the state-system $(S)_\varepsilon$ admits a unique solution $[\eta, \theta]$, defined as follows.

$$(S0) \quad [\eta, \theta] = \{[\eta_i]_{i=1}^n, [\theta_i]_{i=1}^n\} \in ([H^2(\Omega)]^n \times [L^\infty(\Omega)]^n) \times [Y_0]^n$$

$$(S1) \quad \frac{1}{\tau}(\eta_i - \eta_{i-1}) - \Delta \eta_i + g(\eta_i) + \alpha'(\eta_i) f_\varepsilon(\nabla \theta_{i-1}) = u_i \text{ in } \Omega,$$

subject to $r_* \leq \eta_i \leq r^*$ a.e. in Ω , $\nabla \eta_i \cdot n_\Gamma = 0$ on Γ , for $i = 1, 2, 3, \dots, n$

$$(S2) \quad \frac{1}{\tau} \alpha_0(\eta_{i-1})(\theta_i - \theta_{i-1}) - \operatorname{div}(\alpha(\eta_i) \omega_i^* + \nu^2 \nabla \theta_i) = v_i \text{ in } \Omega,$$

with $\omega_i^* \in L^\infty(\Omega)$ satisfying $\omega_i^* \in \partial f_\varepsilon(\nabla \theta_i)$ a.e. in Ω ,

subject to $\theta_i = 0$ on Γ , for $i = 1, 2, 3, \dots, n$

* $f_\varepsilon(\omega) := \sqrt{\varepsilon^2 + |\omega|^2}, \forall \omega \in \mathbb{R}, \varepsilon > 0$ ($f_\varepsilon \rightarrow |\cdot|$ in $L^\infty(\mathbb{R})$ as $\varepsilon \downarrow 0$)

* the case when $\varepsilon = 0, \omega_i^* \in \operatorname{Sgn}(\nabla \theta_i)$ a.e. in Ω

* $\operatorname{Sgn} : \omega \in \mathbb{R}^N \rightarrow \operatorname{Sgn}(\omega) \{ \omega^* \in \mathbb{R}^N : \omega^* \cdot (z - \omega) \leq |z| - |\omega|, \forall z \in \mathbb{R}^N \}$ set-valued sign function

†. cf. [Moll–S.–Watanabe](2015): If $[u, v] = \{[u_i]_{i=1}^n, [v_i]_{i=1}^n\} = 0$ in $[\mathbb{X}]^2$, then we further verify **energy-dissipation** for the following sequence of **free-energy**:

$$\left\{ \mathcal{F}_i \right\}_{i=1}^n := \left\{ \frac{1}{2} \int_\Omega |\nabla \eta_i|^2 dx + \int_\Omega G(\eta_i) dx + \int_\Omega \alpha(\eta_i) |\nabla \theta_i| dx + \frac{\nu^2}{2} \int_\Omega |\nabla \theta_i|^2 dx \right\}_{i=1}^n$$

Proposition 2 (Continuous dependence for the state-system $(S)_\varepsilon$) cf. [Kubota–S.](2020–)

Under (A0)–(A5), let us define:

$$\mathcal{S}_\varepsilon : [u, v] \in \mathcal{U}_{\text{ad}} \mapsto [\eta_\varepsilon, \theta_\varepsilon] := \mathcal{S}_\varepsilon[u, v] : \text{the solution to } (S)_\varepsilon, \text{ for } \varepsilon \geq 0$$

Then,

$$\begin{aligned} & \{\varepsilon_m\}_{m=1}^\infty \subset [0, 1], \varepsilon_m \rightarrow \varepsilon, [u_m, v_m] \rightarrow [u, v] \text{ weakly in } [\mathbb{X}]^2, \text{ as } m \rightarrow \infty \\ \implies & [\eta_m, \theta_m] := \mathcal{S}_{\varepsilon_m}[u_m, v_m] \rightarrow [\eta, \theta] := \mathcal{S}_\varepsilon[u, v] \text{ in } [Y]^n \times [Y_0]^n, \text{ as } m \rightarrow \infty \end{aligned}$$

Theorem A (Existence and parameter dependence of optimal controls)

(I) Under (A0)–(A5) $\varepsilon \geq 0$, the following two items holds.

The problem $(OP)_\varepsilon$ admits at least one optimal control $[u_\varepsilon^*, v_\varepsilon^*] \in \mathcal{U}_{\text{ad}}$

(II) Under (A0)–(A5) $\varepsilon_0 \geq 0$, let $\{[u_\varepsilon^*, v_\varepsilon^*]\}_{\varepsilon \geq 0}$ be a sequence optimal controls

$$\exists \{\varepsilon_m\}_{m=1}^\infty \subset \{\varepsilon\}_{\varepsilon \geq 0}, \exists [u^*, v^*] \in \mathcal{U}_{\text{ad}} \text{ s.t. :}$$

$$\begin{cases} \varepsilon_m \rightarrow \varepsilon_0, [u_{\varepsilon_m}^*, v_{\varepsilon_m}^*] \rightarrow [u^*, v^*] \text{ weakly in } [\mathbb{X}]^2 \text{ as } m \rightarrow \infty, \\ [u^*, v^*]: \text{optimal control of } (OP)_{\varepsilon_0} \end{cases}$$

†. Theorem A will be obtained as a consequence of the argument of **minimizing sequence**

◇ Adjoint of the linearized state-system (necessary condition of optimality)

Adjoint system (A) $_{\varepsilon}$ ($\varepsilon > 0$): to find $[p, z] = [\{p_i\}_{i=1}^n, \{z_i\}_{i=1}^n] \in [\mathbb{X}]^2$ s.t.

$$\left\{ \begin{array}{l} \frac{p_i - p_{i+1}}{\tau} - \Delta p_i + \mu_i p_i + \lambda_i p_i + \omega_i \cdot \nabla z_i + \tilde{\lambda}_i z_i = h_i, \text{ in } \Omega, \quad (\text{ad.1}) \\ \frac{a_i z_i - a_{i+1} z_{i+1}}{\tau} - \operatorname{div} (A_i \nabla z_i + \nu \nabla z_i + p_{i+1} \tilde{\omega}_i) = k_i, \text{ in } \Omega, \quad (\text{ad.2}) \\ \nabla p_i \cdot n_{\Gamma} = z_i = 0, \text{ on } \Gamma, \end{array} \right.$$

for $i = n, \dots, 3, 2, 1$, with $[p_{n+1}, z_{n+1}] = [0, 0]$ in Ω

In this context,

$[h, k] = [\{h_i\}_{i=1}^n, \{k_i\}_{i=1}^n] \in [\mathbb{X}]^2$: forcing, $[\eta_{\varepsilon}, \theta_{\varepsilon}] = [\{\eta_{\varepsilon, i}\}_{i=1}^n, \{\theta_{\varepsilon, i}\}_{i=1}^n]$: sol. to (S) $_{\varepsilon}$

$$\left\{ \begin{array}{l} a_i = \alpha_0(\eta_{\varepsilon, i-1}), \mu_i = \alpha''(\eta_{\varepsilon, i}) f_{\varepsilon}(\nabla \theta_{\varepsilon, i-1}), \lambda_i = g'(\eta_i), \omega_i = \alpha'(\eta_{\varepsilon, i}) \nabla f_{\varepsilon}(\nabla \theta_{\varepsilon, i}), \\ A_i = \alpha(\eta_{\varepsilon, i}) \nabla^2 f_{\varepsilon}(\nabla \theta_{\varepsilon, i}), \tilde{\omega}_i = \alpha'(\eta_{\varepsilon, i+1}) \nabla f_{\varepsilon}(\nabla \theta_{\varepsilon, i}), \tilde{\lambda}_i = \alpha'_0(\eta_{\varepsilon, i}) \frac{\theta_{\varepsilon, i} - \theta_{\varepsilon, i-1}}{\tau}, \end{array} \right. \quad i = n, \dots, 3, 2, 1$$

Keypoint: • $N \in \{1, 2, 3, 4\} \implies H^1(\Omega) \subset L^4(\Omega) \implies 0 \leq \mu_i \in X$ and $p_i \in Y$ imply $\mu_i p_i \in H^1(\Omega)^*$

- (ad.1)(ad.2) are **backward scheme**, for the time-step $i = n, \dots, 3, 2, 1$, with the **zero-terminal condition**
- adjoint system (A) $_{\varepsilon}$ is solved **separately**, in the order of (ad.2) \rightarrow (ad.1)
- the time-step-size τ is a **fixed constant**

Theorem B (Necessary condition of optimality in regular problem $(OP)_\varepsilon$ for $\varepsilon > 0$)

Under (A0)–(A5), let $\varepsilon > 0$ and $[u_\varepsilon^*, v_\varepsilon^*] \in \mathcal{U}_{\text{ad}}$ be the optimal control for $(OP)_\varepsilon$. Then, it holds that:

$$(u_\varepsilon^* + p_\varepsilon^*, h - u_\varepsilon^*)_{\mathbb{X}} \geq 0, \quad \forall h \in \mathcal{U}_{\text{ad}} \quad (\sigma_{*,i} \leq h_i \leq \sigma_i^*) \quad \text{and} \quad v_\varepsilon^* + z_\varepsilon^* = 0 \quad \text{in} \quad \mathbb{X}$$

In the context, $[\eta_\varepsilon^*, \theta_\varepsilon^*] := \mathcal{S}_\varepsilon[u_\varepsilon^*, v_\varepsilon^*]$ in $[\mathbb{X}]^2$ and $[p_\varepsilon^*, z_\varepsilon^*] \in [\mathbb{X}]^2$ is a unique solution to:

$$\left\{ \begin{array}{l} \frac{1}{\tau}(p_{\varepsilon,i}^* - p_{\varepsilon,i+1}^*) - \Delta p_{\varepsilon,i}^* + (g'(\eta_{\varepsilon,i}^*) + \alpha''(\eta_{\varepsilon,i}^*)f_\varepsilon(\nabla\theta_{\varepsilon,i-1}^*))p_{\varepsilon,i}^* + \alpha'(\eta_{\varepsilon,i}^*)[\nabla f_\varepsilon](\nabla\theta_{\varepsilon,i}^*) \cdot \nabla z_{\varepsilon,i}^* \\ \quad + \frac{1}{\tau}\alpha'_0(\eta_{\varepsilon,i}^*)(\theta_{\varepsilon,i+1}^* - \theta_{\varepsilon,i}^*)z_{\varepsilon,i+1}^* = \eta_{\varepsilon,i}^* - \eta_{\text{ad},i} \quad \text{in } \Omega, \\ \frac{1}{\tau}(\alpha_0(\eta_{\varepsilon,i-1}^*)z_{\varepsilon,i}^* - \alpha_0(\eta_{\varepsilon,i}^*)z_{\varepsilon,i+1}^*) - \text{div}(\alpha(\eta_{\varepsilon,i}^*)[\nabla^2 f_\varepsilon](\nabla\theta_{\varepsilon,i}^*)\nabla z_{\varepsilon,i}^* \\ \quad + \nu^2\nabla z_{\varepsilon,i}^* + \alpha'(\eta_{\varepsilon,i+1}^*)p_{\varepsilon,i+1}^*[\nabla f_\varepsilon](\nabla\theta_{\varepsilon,i}^*)) = \theta_{\varepsilon,i}^* - \theta_{\text{ad},i} \quad \text{in } \Omega, \\ \nabla p_{\varepsilon,i}^* \cdot n_\Gamma = 0, \quad z_{\varepsilon,i}^* = 0 \quad \text{on } \Gamma, \quad \text{for any } i = n, \dots, 3, 2, 1, \\ p_{\varepsilon,n+1}^* = z_{\varepsilon,n+1}^* = 0, \quad \text{in } \Omega. \end{array} \right.$$

Keypoint:

- the temperature $u = \{u_i\}_{i=1}^n \in [\mathbb{X}]^2$ is **constrained on \mathcal{U}_{ad}**
 \implies the necessary condition for the 1st component u is obtained as a **variational inequality**
- there is no constraint for the component $v = \{v_i\}_{i=1}^n \in [\mathbb{X}]^2$
 \implies the necessary condition for the 2nd component v is obtained as an **equality**

Theorem B (Necessary condition of optimality in regular problem $(\text{OP})_\varepsilon$ for $\varepsilon > 0$)

Under (A0)–(A5), let $\varepsilon > 0$ and $[u_\varepsilon^*, v_\varepsilon^*] \in \mathcal{U}_{\text{ad}}$ be the optimal control for $(\text{OP})_\varepsilon$. Then, it holds that:

$$(u_\varepsilon^* + p_\varepsilon^*, h - u_\varepsilon^*)_{\mathbb{X}} \geq 0, \quad \forall h \in \mathcal{U}_{\text{ad}} \quad (\sigma_{*,i} \leq h_i \leq \sigma_i^*) \quad \text{and} \quad v_\varepsilon^* + z_\varepsilon^* = 0 \quad \text{in} \quad \mathbb{X}$$

In the context, $[\eta_\varepsilon^*, \theta_\varepsilon^*] := \mathcal{S}_\varepsilon[u_\varepsilon^*, v_\varepsilon^*]$ in $[\mathbb{X}]^2$ and $[p_\varepsilon^*, z_\varepsilon^*] \in [\mathbb{X}]^2$ is a unique solution to:

$$u_{\varepsilon,i}^*(x) = \text{proj}_{[\sigma_{*,i}(x), \sigma_i^*(x)]}(-p_{\varepsilon,i}^*(x)) = \begin{cases} -p_{\varepsilon,i}^*(x), & \text{if } \sigma_{*,i}(x) \leq -p_{\varepsilon,i}^*(x) \leq \sigma_i^*(x) \\ \sigma_i^*(x), & \text{if } -p_{\varepsilon,i}^*(x) \geq \sigma_i^*(x) \\ \sigma_{*,i}(x), & \text{if } -p_{\varepsilon,i}^*(x) \leq \sigma_{*,i}(x) \end{cases}$$

a.e. $x \in \Omega$, $i = n, \dots, 3, 2, 1$

- for $-\infty \leq a < b \leq \infty$, $\text{proj}_{[a,b]} : \mathbb{R} \rightarrow [a,b] \cap \mathbb{R}$ is the projection on to $[a,b] \cap \mathbb{R}$

Keypoint:

- the temperature $u = \{u_i\}_{i=1}^n \in [\mathbb{X}]^2$ is **constrained on \mathcal{U}_{ad}**
 \implies the necessary condition for the 1st component u is obtained as a **variational inequality**
- there is no constraint for the component $v = \{v_i\}_{i=1}^n \in [\mathbb{X}]^2$
 \implies the necessary condition for the 2nd component v is obtained as an **equality**

Theorem C (Limiting observation of necessary condition for $(\text{OP})_\varepsilon$, as $\varepsilon \downarrow 0$)

Under (A0)–(A5), there exist an optimal control $[u^\circ, v^\circ] \in \mathcal{U}_{\text{ad}}$ for $(\text{OP})_0$, $[\eta^\circ, \theta^\circ] = \mathcal{S}_0[u^\circ, v^\circ]$, and $[\xi^\circ, \zeta^\circ, \omega^\circ] = \{[\xi_i^\circ]_{i=1}^n, [\zeta_i^\circ]_{i=1}^n, [\omega_i^\circ]_{i=1}^n\} \in \mathbb{X} \times [H^{-1}(\Omega)]^n \times [L^\infty(\Omega)]^n$, s.t.:

$$(u^\circ + p^\circ, h - u^\circ)_\mathbb{X} \geq 0, \quad \forall h \in \mathcal{U}_{\text{ad}} \quad (\sigma_{*,i} \leq h_i \leq \sigma_i^*), \quad v^\circ + z^\circ = 0 \quad \text{in } \mathbb{X},$$

$$\text{and } \omega_i^\circ \in \text{Sgn}(\nabla \theta_i^\circ) \text{ a.e. in } \Omega,$$

$$\begin{cases} \frac{1}{\tau}(p_i^\circ - p_{i+1}^\circ) - \Delta p_i^\circ + (g'(\eta_i^\circ) + \alpha''(\eta_i^\circ)|\nabla \theta_{i-1}^\circ|)p_i^\circ + \alpha'(\eta_i^\circ)\xi_i^\circ \\ \quad + \frac{1}{\tau}\alpha'_0(\eta_i^\circ)(\theta_{i+1}^\circ - \theta_i^\circ)z_{i+1}^\circ = \eta_i^\circ - \eta_{\text{ad},i} \quad \text{in } X, \\ \frac{1}{\tau}(\alpha_0(\eta_{i-1}^\circ)z_i^\circ - \alpha_0(\eta_i^\circ)z_{i+1}^\circ) + \zeta_i^\circ - \text{div}(\nu^2 \nabla z_i^\circ + \alpha'(\eta_{i+1}^\circ)\omega_i^\circ p_{i+1}^\circ) = \theta_i^\circ - \theta_{\text{ad},i} \quad \text{in } H^{-1}(\Omega) = Y_0^*, \\ \nabla p_i^\circ \cdot n_\Gamma = 0, \quad z_i^\circ = 0 \quad \text{on } \Gamma, \text{ for any } i = n, \dots, 3, 2, 1, \\ p_{n+1}^\circ = z_{n+1}^\circ = 0, \quad \text{in } \Omega. \end{cases}$$

Keypoint: • $\xi_i^\circ \sim \frac{D\theta_i^\circ}{|D\theta_i^\circ|} \cdot \nabla z_i^\circ$, $\zeta_i^\circ \sim -\text{div}(\alpha(\eta_i^\circ)[\nabla \text{Sgn}] (\nabla \theta_i^\circ) \nabla z_i^\circ)$

- estimate of perturbed Poisson eq. to have **strong convergence** $p_\varepsilon^* \rightarrow p^\circ$ in \mathbb{X} (H^1 -boundedness) \implies we obtain the limiting necessary condition of **variational inequality**
- the necessary condition of **equality**, and the **linearity** of adjoint system \implies we need only weak-convergences $p_\varepsilon^* \rightarrow p^\circ$ weakly in Y , $z_\varepsilon^* \rightarrow z^\circ$ weakly in Y_0 (H^1 -boundedness)

5. Precise observation in 1D case

$\Omega := (0, 1) \subset \mathbb{R}$ (1D-domain), $\Gamma = \partial\Omega = \{0, 1\}$, $X := L^2(\Omega)$, $\mathbb{X} := [X]^n$

Problem (OP) $_{\varepsilon}$ ($\varepsilon \geq 0$): to find $[u^*, v^*] = [\{u_i^*\}_{i=1}^n, \{v_i^*\}_{i=1}^n] \in [\mathbb{X}]^2$, called **optimal control**, s.t.

$$[u^*, v^*] = \arg\text{-min} \mathcal{J}_{\varepsilon} = \mathcal{J}_{\varepsilon}(u, v) \text{ on } [\mathbb{X}]^2 \text{ (constraint-free setting),}$$

with a cost functional $\mathcal{J} : [u, v] \in [\mathbb{X}]^2 \mapsto \mathcal{J}(u, v) \in [0, \infty)$, defined as

$$\mathcal{J}(u, v) := \frac{1}{2} |[\eta, \theta] - [\eta_{\text{ad}}, \theta_{\text{ad}}]|_{[\mathbb{X}]^2}^2 + \frac{1}{2} |[u, v]|_{[\mathbb{X}]^2}^2.$$

State-system (S) $_{\varepsilon}$:

$$\begin{cases} \frac{1}{\tau}(\eta_i - \eta_{i-1}) - \partial_x^2 \eta_i + g(\eta_i) + \alpha'(\eta_i) |\partial_x \theta_{i-1}| = u_i \text{ in } \Omega, \\ \frac{1}{\tau} \alpha_0(\eta_{i-1})(\theta_i - \theta_{i-1}) - \partial_x(\alpha(\eta_i) \partial f_{\varepsilon}(\partial_x \theta_i) + \nu^2 \partial_x \theta_i) \ni v_i \text{ in } \Omega, \\ \partial_x \eta_i = \theta_i = 0 \text{ on } \Gamma, i = 1, 2, 3, \dots, n, \\ \eta_0 \in H^1(\Omega), \theta_0 \in H_0^1(\Omega). \end{cases}$$

†. The **one-dimensional embedding** $H^1(\Omega) \subset C(\overline{\Omega})$ enables to remove the constraint for the temperature $u = \{u_i\}_{i=1}^n \in \mathbb{X}$

Proposition 3 (cf. [Rybka, Mucha](2013), [Kubota](2021))

Let us fix $0 \leq \beta_1 \in Y$ and $0 < \beta_2 \in Y$, and let us set the three convex functionals V_{β_1} , W_{β_2} , and Φ_{β_1, β_2} , defined as follows, respectively:

$$z \in X \mapsto V_{\beta_1}(z) := \sup \left\{ \int_{\Omega} z \partial_x \varphi \, dx \mid \begin{array}{l} \varphi \in Y \cap C_c(\Omega), \text{ such that} \\ |\varphi| \leq \beta_1 \text{ on } \bar{\Omega} \end{array} \right\} \sim \int_{\Omega} \beta_1 |\partial_x z|,$$

$$z \in X \mapsto W_{\beta_2}(z) := \begin{cases} \frac{1}{2} \int_{\Omega} \beta_2 |\partial_x z|^2 \, dx, & \text{if } z \in Y, \\ \infty, & \text{otherwise,} \end{cases}$$

$$z \in X \mapsto \Phi_{\beta_1, \beta_2}(z) := V_{\beta_1}(z) + W_{\beta_2}(z).$$

Then, the subdifferential $\partial\Phi_{\beta_1, \beta_2} \subset X \times X$ of the convex function Φ_{β_1, β_2} is decomposed as follows:

$$\partial\Phi_{\beta_1, \beta_2} = \partial V_{\beta_1} + \partial W_{\beta_2} \text{ in } X \times X.$$

†₁. Applying this Proposition to the case when $\beta_1 = \alpha(\eta_i)$, $\beta_2 \equiv \nu^2$,

$\theta_i \in H^2(\Omega)$, and $-\partial_x(\alpha(\eta_i)\omega_i^* + \nu^2 \partial_x \theta_i) = -\partial_x(\alpha(\eta_i)\omega_i^*) - \nu^2 \partial_x^2 \theta_i$ in X , with $\omega_i^* \in \partial f_{\varepsilon}(\partial_x \theta_i)$ a.e. in Ω .

Proposition 4 (H^2 -regularity of the solution θ)

(I) Under (A0)–(A5), $\varepsilon \geq 0$ and $[u, v] \in [\mathbb{X}]^2$, the state-system $(S)_\varepsilon$ admits a unique solution $[\eta, \theta]$, defined as follows:

$$(S0) \quad \eta_i \in H^2(\Omega) \text{ and } \theta_i \in H^2(\Omega), i = 1, 2, 3, \dots, n$$

$$(S1) \quad \frac{1}{\tau}(\eta_i - \eta_{i-1}) - \partial_x^2 \eta_i + g(\eta_i) + \alpha'(\eta_i) f_\varepsilon(\partial_x \theta_{i-1}) = u_i \text{ in } \Omega,$$

subject to $\partial_x \eta_i = 0$ on Γ , for any $i = 1, 2, 3, \dots, n$, and $\eta_0 \in Y$

$$(S2) \quad \frac{1}{\tau} \alpha_0(\eta_{i-1})(\theta_i - \theta_{i-1}) - \partial_x(\alpha(\eta_i) \omega_i^*) - \nu^2 \partial_x^2 \theta_i = v_i \text{ in } \Omega,$$

with $\omega_i^* \in Y \cap L^\infty(\Omega)$ satisfying $\omega_i^* \in \partial f_\varepsilon(\partial_x \theta_i)$ a.e. in Ω ,

subject to $\theta_i = 0$ on Γ , for any $i = 1, 2, 3, \dots, n$, and $\theta_0 \in Y_0$

(II) Under (A0)–(A5), let us define:

$$\mathcal{S}_\varepsilon : [u, v] \in [\mathbb{X}]^2 \mapsto [\eta_\varepsilon, \theta_\varepsilon] := \mathcal{S}_\varepsilon[u, v] : \text{the solution to } (S)_\varepsilon, \text{ for } \varepsilon \geq 0$$

Then,

$$\begin{aligned} & \{\varepsilon_m\}_{m=1}^\infty \subset (0, 1], \varepsilon_m \rightarrow \varepsilon, [u_m, v_m] \rightarrow [u, v] \text{ weakly in } [\mathbb{X}]^2, \text{ as } m \rightarrow \infty \\ \implies & [\eta_m, \theta_m] := \mathcal{S}_{\varepsilon_m}[u_m, v_m] \rightarrow [\eta, \theta] := \mathcal{S}_\varepsilon[u, v] \text{ in } ([Y]^n \cap [C^1(\bar{\Omega})]^n) \times ([Y_0]^n \cap [C^1(\bar{\Omega})]^n), \\ & \text{and weakly in } [H^2(\Omega)]^n \times [H^2(\Omega)]^n \quad (\partial_x \theta_m \rightarrow \partial_x \theta \text{ in } C(\bar{\Omega})), \text{ as } m \rightarrow \infty \end{aligned}$$

Theorem D (A precise characterization of the limiting necessary condition of optimality)

Under (A0)–(A5), there exist an optimal control $[u^\circ, v^\circ] \in [\mathbb{X}]^2$ for (OP)₀, $[\eta^\circ, \theta^\circ] = \mathcal{S}_0[u^\circ, v^\circ]$, and $[\xi^\circ, \zeta^\circ, \omega^\circ] = \{[\xi_i^\circ]_{i=1}^\circ, [\zeta_i^\circ]_{i=1}^\circ, [\omega_i^\circ]_{i=1}^\circ\} \in \mathbb{X} \times [H^{-1}(\Omega)]^n \times [L^\infty(\Omega)]^n$, s.t.:

$$\begin{aligned} & [u^\circ, v^\circ] = -[p^\circ, z^\circ] \text{ in } [\mathbb{X}]^2 \text{ and } \omega_i^\circ \in \text{Sgn}(\partial_x \theta_i^\circ) \text{ a.e. in } \Omega, \\ & \begin{cases} \frac{1}{\tau}(p_i^\circ - p_{i+1}^\circ) - \partial_x^2 p_i^\circ + (g'(\eta_i^\circ) + \alpha''(\eta_i^\circ)|\partial_x \theta_{i-1}^\circ|)p_i^\circ + \alpha'(\eta_i^\circ)\xi_i^\circ \\ \quad + \frac{1}{\tau}\alpha'_0(\eta_i^\circ)(\theta_{i+1}^\circ - \theta_i^\circ)z_{i+1}^\circ = \eta_i^\circ - \eta_{\text{ad},i} \text{ in } \Omega, \\ \frac{1}{\tau}(\alpha_0(\eta_{i-1}^\circ)z_i^\circ - \alpha_0(\eta_i^\circ)z_{i+1}^\circ) + \zeta_i^\circ - \partial_x(\nu^2 \partial_x z_i^\circ + \alpha'(\eta_{i+1}^\circ)\omega_i^\circ p_{i+1}^\circ) = \theta_i^\circ - \theta_{\text{ad},i} \text{ in } \Omega, \\ \partial_x p_i^\circ = z_i^\circ = 0 \text{ on } \Gamma, \text{ for any } i = n, \dots, 3, 2, 1, \quad p_{n+1}^\circ = z_{n+1}^\circ = 0, \text{ in } \Omega. \end{cases} \end{aligned}$$

Keypoints: Under 1D-setting,

- the distribution ζ° is formally expressed by:

$$\zeta_i^\circ \sim -\partial_x [\alpha(\eta_i) \mathfrak{D}(\partial_x \theta_i^\circ) \partial_x v_i^\circ] \text{ in } \mathcal{D}'(\Omega), \text{ and } \text{spt} \zeta_i^\circ \sim \{\partial_x \theta_i^\circ = 0\}, \text{ by using Dirac's delta } \mathfrak{D}$$

- as $\varepsilon \downarrow 0$, the limiting component $\partial_x \theta^\circ \in C(\overline{\Omega})$ is approached in the **uniform topology on $\overline{\Omega}$**
- the set $\{\partial_x \theta_i^\circ = 0\}$ corresponds to a **closed region** of locally constant parts (**crystalline facets on grains**)
the set $\{\partial_x \theta_i^\circ \neq 0\}$ is an **open set**, corresponding to a **neighborhood of grain boundary**

Theorem D (A precise characterization of the limiting necessary condition of optimality)

Let us take any $\rho \in C^1(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$ with $\rho(0) = \rho'(0) = 0$. Then,

$$\rho(\partial_x \theta_i^\circ) \left(\frac{1}{\tau} (p_i^\circ - p_{i+1}^\circ) - \partial_x^2 p_i^\circ + (g'(\eta_i^\circ) + \alpha''(\eta_i^\circ) |\partial_x \theta_{i-1}^\circ|) p_i^\circ + \alpha'(\eta_i^\circ) \omega_i^\circ \partial_x z_i^\circ \right. \\ \left. + \frac{1}{\tau} \alpha'_0(\eta_i^\circ) (\theta_{i+1}^\circ - \theta_i^\circ) z_{i+1}^\circ - (\eta_i^\circ - \eta_{\text{ad},i}) \right) = 0 \text{ in } X,$$

$$\rho(\partial_x \theta_i^\circ) \left(\frac{1}{\tau} (\alpha_0(\eta_{i-1}^\circ) z_i^\circ - \alpha_0(\eta_i^\circ) z_{i+1}^\circ) - \nu^2 \partial_x^2 z_i^\circ - \alpha'(\eta_{i+1}^\circ) \omega_i^\circ p_{i+1}^\circ - (\theta_i^\circ - \theta_{\text{ad},i}) \right) = 0 \text{ in } X,$$

$\xi_i^\circ = \omega_i^\circ \partial_x z_i^\circ$ and $\zeta_i^\circ = 0$ in $\mathcal{D}'(\{\partial_x \theta_i^\circ \neq 0\})$, with $\omega_i^\circ \in \text{Sgn}(\nabla \theta_i^\circ)$ in Ω , for $i = n, \dots, 3, 2, 1$.

Therefore,

$$\begin{cases} \frac{1}{\tau} (p_i^\circ - p_{i+1}^\circ) - \partial_x^2 p_i^\circ + (g'(\eta_i^\circ) + \alpha''(\eta_i^\circ) |\partial_x \theta_{i-1}^\circ|) p_i^\circ + \alpha'(\eta_i^\circ) \frac{\partial_x \theta_i^\circ}{|\partial_x \theta_i^\circ|} \partial_x z_i^\circ \\ \quad + \frac{1}{\tau} \alpha'_0(\eta_i^\circ) (\theta_{i+1}^\circ - \theta_i^\circ) z_{i+1}^\circ = \eta_i^\circ - \eta_{\text{ad},i}, \\ \frac{1}{\tau} (\alpha_0(\eta_{i-1}^\circ) z_i^\circ - \alpha_0(\eta_i^\circ) z_{i+1}^\circ) - \nu^2 \partial_x^2 z_i^\circ - \alpha'(\eta_{i+1}^\circ) \frac{\partial_x \theta_i^\circ}{|\partial_x \theta_i^\circ|} p_{i+1}^\circ = \theta_i^\circ - \theta_{\text{ad},i}, \end{cases} \quad \text{in } \{\partial_x \theta_i^\circ \neq 0\}$$

◇ **Sketch of the proof (2nd eq. of the adjoint system):**

$\forall i \in \{1, \dots, n\}$, let us take $\psi \in Y_0$, and **test 2nd eq. by $\rho(\partial_x \theta_i^\circ) \psi \in Y_0$ ($\theta_i^\circ \in H^2(\Omega)$):**

$$\begin{aligned}
 \text{(principal part) } I_\varepsilon^\circ &:= \int_{\Omega} (\alpha(\eta_{\varepsilon,i}^*) f_\varepsilon''(\partial_x \theta_{\varepsilon,i}^*) \partial_x z_{\varepsilon,i}^*) \cdot \partial_x (\rho(\partial_x \theta_i^\circ) \psi) \, dx \\
 &= \int_{\text{spt} \rho(\partial_x \theta_i^\circ)} \partial_x z_{\varepsilon,i}^* \cdot \boxed{\alpha(\eta_{\varepsilon,i}^*) \frac{\varepsilon^2}{\sqrt{\varepsilon^2 + |\partial_x \theta_{\varepsilon,i}^*|^2}^3} (\rho'(\partial_x \theta_i^\circ) \partial_x^2 \theta_i^\circ \psi + \rho(\partial_x \theta_i^\circ) \partial_x \psi)} \, dx \\
 &\hspace{15em} (*1)_\varepsilon
 \end{aligned}$$

(Step 1): the case when $0 \notin K^\circ := \text{spt} \rho$, i.e. $\exists \delta^\circ > 0$ s.t. $K^\circ \cap (-\delta^\circ, \delta^\circ) = \emptyset$

- **uniform convergence on $\bar{\Omega}$ of $\eta_{\varepsilon,i}^* \rightarrow \eta_i^\circ$, and $\partial_x \theta_{\varepsilon,i}^* \rightarrow \partial_x \theta_i^\circ$:**

$\exists \varepsilon^\circ > 0$ s.t. $|\partial_x \theta_{\varepsilon,i}^*| \geq \delta^\circ/2$, **uniformly on $\text{spt} \rho(\partial_x \theta_i^\circ)$** , $\forall \varepsilon \in (0, \varepsilon^\circ)$

$$\implies |(*1)_\varepsilon|_X \leq \text{Const.} \frac{\varepsilon^2}{\sqrt{\varepsilon^2 + |\partial_x \theta_{\varepsilon,i}^*|^2}^3} (|\partial_x^2 \theta_i^\circ|_X + |\partial_x \psi|_X) \leq \text{Const.} \frac{2}{\delta^\circ} (|\partial_x^2 \theta_i^\circ|_X + |\partial_x \psi|_X) \rightarrow 0, \text{ as } \varepsilon \downarrow 0$$

$$\implies I_\varepsilon^\circ \rightarrow 0, \text{ as } \varepsilon \downarrow 0$$

(Step 2): the case when $0 \in K^\circ := \text{spt} \rho$ ($\rho(0) = \rho'(0) = 0$)

This case is obtained by means of approximating argument of ρ in $W^{1,\infty}(\mathbb{R})$ □

6. Future problems

(I) Optimal control problems for anisotropic Kobayashi–Warren–Carter system

Issue : 2D state-system with crystalline anisotropy

(II) Optimal control problems for WKLC system (cf. [Warren–Kobayashi–Lobkovsky–Carter] (2003))

Issue : state-system of “Fix–Caginalp model of phase transition” VS.
“Kobayashi–Warren–Carter system”

(III) Generalization of boundary conditions

Issue : unification of the methods for nonhomogeneous Dirichlet / Neumann / Robin B.C., and dynamic B.C.

(IV) Issues for time-discrete state-systems in higher dimension

Issue : expression of ξ_i° and ζ_i°